Unsupervised Analysis: Introduction

About the Instructors

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- Rice University - Departments of Statistics, CS, and ECE & Baylor College of Medicine - Neurological Research Institute.
- Research:
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  http://www.stat.rice.edu/~gallen/

- Fun facts. . .

About the Instructors

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- University of North Carolina, Chapel Hill - Departments of Statistics and Operations Research, Genetics, & Biostatistics.
- Research:
  - Statistical Machine Learning and Data Mining; High-dimensional Data Analysis; Nonparametric Statistics and Functional Estimation; Bioinformatics; Design and Analysis of Experiments.

  `http://www.unc.edu/~yfliu/`
- Fun facts. . .

Statistical Machine Learning

- "Learn" from current data to make predictions about the future.

  Examples?

- Intersection of: Computer Science, Statistics, Applied Math.

Big Data

Big Data - BIG in Volume, Variety and/or Velocity (or Complexity!).

Common Big Data themes in Statistical Learning:

- Big n. Large number of observations.
  - Examples: Internet data, financial transactions, climate data, etc.
- Big p. Large number of features relative to observations. (High-dimensional data).
  - Examples: Medical data - genomics, neuroimaging, medical imaging, etc.

Big Biomedical Data

Examples:

- High-throughput Genomics ("Omics").
  - RNA-sequencing, microarrays, methylation arrays, CGH-arrays, exome sequencing, mass spectrometry, NMR spectroscopy, etc.
- Neuroimaging / neural recordings.
  - MRI, Functional MRI (fMRI), EEG, MEG, DTI, ECoG, PET, etc.
- Electronic Health Records.
- Medical Imaging.

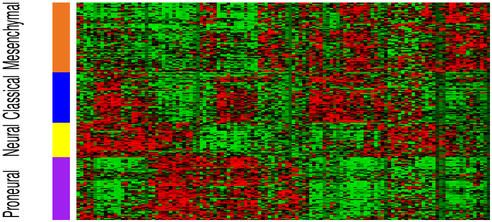
Data Matrix

Data Matrix:

$$\boldsymbol{X}_{n\times p} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ \vdots & & \ddots & \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}$$

- Rows: n observations / samples / subjects.
- Columns: p features / variables.

Example: Omics Data



Gene Expression Data

Unsupervised vs. Supervised Learning

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Supervised Learning:

$$\mathbf{y} = (y_1, y_2, \dots y_n)^T$$

- $\mathbf{y}$ - n labels / outcomes associated with each observation.

Unsupervised Learning: No outcomes / labels!

Supervised Learning

Main Goal

Prediction!

- Given: $(Y_n^{train}, \boldsymbol{X}_{n \times p}^{train})$ (Training Data).
- Training: Use training data to find $\hat{f}()$ that maps $\boldsymbol{X}$ to Y: $Y = \hat{f}(\boldsymbol{X}) + \epsilon$.
- Prediction: Given new $\boldsymbol{X}_{m \times p}^{test}$, predict $Y_{m \times 1}^{test}$: $\hat{Y}^{test} = \hat{f}(\boldsymbol{X}^{test})$.

Examples?

Secondary Goals:

- Feature Selection - What features are associated with the outcome?
- Others?

Unsupervised Learning

No labels! What is the goal?

Main Goal

Find some structure that characterizes the data.

(Or, find structure in training data that we expect to be present in future data.)

- Find patterns. (PCA, ICA, NMF, MDS)
- Dimension reduction. (PCA)
- Group observations / Group features / Group both. (Clustering)
- Find associations / relationships between features or observations. (Graphical or Network Models)
- Filter features. (Association testing)

Unsupervised Learning

Challenges:

- Difficult to validate unsupervised learning results.
- No validation or test labels to measure prediction accuracy.
- What is meaningful structure in data?

Uses:

- Data pre-processing / compression / denoising.
- Exploratory data analysis.
  - Need to use multiple unsupervised learning techniques as each gives slightly different "insights" into data.
- Data visualization.

Unsupervised Learning

How is it used in Big Biomedical Data?

Case Study: BRCA gene expression data.

- Data Visualization.
  - Cluster heatmap, graphical models, MDS, PCA.
- Exploratory Analysis.
  - Clustering / dimension reduction to find cancer subtypes.
- Gene Selection.
  - Large-scale hypothesis testing to find genes associated with subtypes.
- Gene Interactions.
  - Graphical models.

This Course

1. Lecture 1 - Dimension Reduction - PCA.
2. Lecture 2 - Dimension Reduction - PCA, NMF, ICA, MDS, Others.
3. Lab 1 - Dimension Reduction.

4. Lecture 3 - Clustering - Intro and K-means.
5. Lecture 4 - Clustering - Hierarchical, and other techniques.
6. Lab 2 - Clustering.

7. Lecture 5 - Graphical Models.
8. Lab 3 / Lecture 6 - Graphical Models Lab & Individualized Treatment Rules.

9. Lecture 7 - Large-Scale Hypothesis Testing & Best Practices.
10. Lab 4 BRCA case study.